

Start Date: Any Date

Total Records Found: 24

End Date: Any Date

Accounting Date	Sequence Num.	Tran Type	Fee Code	Fee Amount	Mailroom Date	Payment Method
07/30/1999	00000052	1	101	\$760.00	07/22/1999	OP
07/30/1999	00000053	1	103	\$4,248.00	07/22/1999	DA 041406
07/30/1999	00000054	1	103	\$1,962.00	07/22/1999	OP
07/30/1999	00000055	1	102	\$1,170.00	07/22/1999	DA 041406
07/30/1999	00000056	1	104	\$260.00	07/22/1999	DA 041406
10/19/1999	00000001	1	101	-\$760.00	07/22/1999	OP
10/19/1999	00000002	1	103	-\$4,248.00	07/22/1999	DA 041406
10/19/1999	00000003	1	103	-\$1,962.00	07/22/1999	OP
10/19/1999	00000004	1	102	-\$1,170.00	07/22/1999	DA 041406
10/19/1999	00000005	1	104	-\$260.00	07/22/1999	DA 041406
10/19/1999	00000006	1	201	\$380.00	07/22/1999	OP
10/19/1999	00000007	1	203	\$763.00	07/22/1999	DA 041406
10/19/1999	00000008	1	203	\$2,342.00	07/22/1999	OP
10/19/1999	00000009	1	202	\$585.00	07/22/1999	DA 041406
10/19/1999	00000010	1	204	\$130.00	07/22/1999	DA 041406
10/19/1999	00000191	1	205	\$65.00	10/18/1999	OP
10/20/1999	00000339	1	581	\$40.00	10/18/1999	OP
11/26/1999	00000004	1	203	-\$763.00	07/22/1999	DA 041406
11/26/1999	00000005	1	203	-\$2,342.00	07/22/1999	OP
11/26/1999	00000006	1	204	-\$130.00	07/22/1999	DA 041406
11/26/1999	00000007	1	203	\$396.00	07/22/1999	OP
11/26/1999	00000008	4	704	-\$1,946.00	07/22/1999	OP
11/20/2000	00000098	1	215	\$55.00	11/16/2000	OP
11/20/2000	00000099	1	203	\$72.00	11/16/2000	OP

387  
+ 9  
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396

	L #	Hit s	Search Text	DBs	Time Stamp
1	L1	796	combinatorial adj library	USPAT	2001/01/1 6 11:31
2	L2	1	static adj filter	USPAT	2001/01/1 6 11:31
3	L3	3	modelling	USPAT	2001/01/1 6 11:32
4	L4	0	1 and 2 and 3	USPAT	2001/01/1 6 11:32
5	L5	40	1 and 3	USPAT	2001/01/1 6 11:33
6	L6	26	5 and computer	USPAT	2001/01/1 6 11:33
7	L7	2	modelling and computer and combinatorial	EPD; JPD; Derwent ; IBM TDB	2001/01/1 6 11:48
8	L8	1	modelling and combinatorial and library	EPD; JPD; Derwent ; IBM TDB	2001/01/1 6 11:48
9	L9	1	filter and combinatorial and library	EPD; JPD; Derwent ; IBM TDB	2001/01/1 6 11:49
10	L10	2	(static or dynamic) and combinatorial and library and model	EPD; JPD; Derwent ; IBM TDB	2001/01/1 6 11:50
11	L11	0	(static or dynamic) and combinatorial and library	EPD; JPD; Derwent ; IBM TDB	2001/01/1 6 11:59
12	L12	486	(static or dynamic) and modelling	EPD; JPD; Derwent ; IBM TDB	2001/01/1 6 11:59

	L #	Hit s	Search Text	DBs	Time Stamp
13	115	5	static or dynamic, and modelling and (molecule or molecules)	EFO; JFC; Berwent ; IBM TDB	0001/00/01 12:00

FILE 'HOME' ENTERED AT 13:15:13 ON 16 JAN 2001

=> index bioscience

FILE 'DRUGMONOG' ACCESS NOT AUTHORIZED

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE ENTRY	FILE SESSION	TOTAL
1.15		1.15

INDEX 'ADISALERTS, ADISINSIGHT, AGRICOLA, ANABSTR, AQUASCI, BIOBUSINESS, BICOMMERCE, BIOSIS, BIOCETHABS, BIOCETHLS, BIOCETHNO, CABAA, CANCERLIT, CAPLUS, CEABA-VTB, CEN, CIN, CONFSCI, CROPB, CROPU, DDFB, DDFU, DGENE, DRUGB, DRUGLAUNCH, DRUGMONOG2, DRUGNL, ...' ENTERED AT 13:15:24 ON 16 JAN 2001

56 FILES IN THE FILE LIST IN STNINDEX

Enter SET DETAIL ON to see search term postings or to view search error messages that display as 0\* with SET DETAIL OFF.

=> s combinatorial library and (static or dynamic) (w) filter and (model or modelling)

16 FILES SEARCHED...

35 FILES SEARCHED...

45 FILES SEARCHED...

0 FILES HAVE ONE OR MORE ANSWERS, 56 FILES SEARCHED IN STNINDEX

LI QUE COMBINATORIAL LIBRARY AND (STATIC OR DYNAMIC) (W) FILTER AND (MODEL OR MODELLING)

=> s (molecule or molecular or dimensional) and (model or modelling) and library and filter?

9 FILE BIOSIS  
7 FILE BIOCETHNO  
1 FILE CABAA  
2 FILE CANCERLIT  
3 FILE CAPLUS

15 FILES SEARCHED...

30 FILE CEN  
7 FILE EMBASE  
5 FILE ESBIOBASE

33 FILES SEARCHED...

5 FILE IFIPAT  
1 FILE LIFESCI  
7 FILE MEDLINE  
49 FILE PRIMT  
9 FILE SCISEARCH  
1 FILE TOXLIT

55 FILES SEARCHED...

205 FILE USPATFULL  
2 FILE WPIDS  
2 FILE WPINDEX

17 FILES HAVE ONE OR MORE ANSWERS, 56 FILES SEARCHED IN STNINDEX

LC QUE (MOLECULE OR MOLECULAR OR DIMENSIONAL) AND (MODEL OR MODELLING) AND LI  
BRARY AND FILTER?

=> d rank

F1	6205	USPATFULL
F2	42	PRCMT
F3	17	CEN
F4	3	BICAF
F5	3	SCISEARCH
F6	7	BICTECHNO
F7	7	EMBASE
F8	7	MEDLINE
F9	6	ESBICBASE
F10	5	IFIPAT
F11	3	CAPLUS
F12	2	CANCERLIT
F13	2	WPIDS
F14	2	WPINDEX
F15	1	CABA
F16	1	LIFESCI
F17	1	TOXLIT

= file f3-f17

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.15	3.30

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FILE 'TOMLIB' ENTERED AT 13:19:23 ON 16 JAN 1974

=\* s l3; dup rem l3

5 FILES SEARCHED...  
12 FILES SEARCHED...  
L3 99 L3

PROCESSING COMPLETED FOR L3  
L4 58 DUP REM L3 .31 DUPLICATES REMOVED.

=\* d 1-59 bib ab; log h

:MATT \*TDB-ACC-NO: NN87023771

DISCLOSURE TITLE: Software Package for Molecular  
Modelling and Structural  
Characterization

PUBLICATION-DATE: IBM Technical Disclosure Bulletin,  
February 1987, US

VOLUME NUMBER: 29

ISSUE NUMBER: 9

PAGE NUMBER: 3771 - 3773

PUBLICATION-DATE: February 1, 1987 (19870201)

CROSS REFERENCE: 0018-8689-29-9-3771

DISCLOSURE TEXT:

- The difficulty in comparing complicated  
molecular structures

and phenomena motivates the development of these  
software packages,

systems, and methods. The highly interactive  
nature of their user

interfaces and the variety of data representations  
available to the

user suggest the extension of these analyses beyond  
the biomolecular

domain. A set of software is disclosed which  
facilitates the

structural and dynamical characterization of  
biomolecules (or other

large molecules). The various routines currently  
run on an IBM 3077

GA and Tektronix Graphics display. The support  
software is PL/I, and

the interactive graphics language is GCS. The  
Random-Dot Display

Program makes use of a moire interference pattern to allow

researchers to compare orientations of structural parts, such as protein subunits.

Method: If a pattern of random dots is superimposed

on itself and rotated by a small angle, concentric circles are

perceived about the point of rotation. If the angle of rotation is

increased, the perceived circles gradually disappear until a totally

unstructured dot display is seen. This effect demonstrates the

ability of the human visual system to detect local autocorrelations

and may suggest a physiological basis of form perception in higher

animals. Demonstration: This graphical technique may be used in

situations where two conformers of a lobed molecule are known and an

equivalent axis of rotation relating the two is desired. First, two

identical random-dot patterns are superimposed over the computer

graphics representation of one form of the protein.

One of the dot

patterns is rotated along with one lobe until the lobe is in its new

position, while the other remains with the stationary lobe. Even a

small change, represented by a one-degree rotation of one lobe

relative to the other, creates a figure where the axis of rotation

can begin to be perceived at the center of the concentric circles.

DNA Spectrogram and Power Spectra - Two useful ways of describing

base content and periodicity for nucleic acid sequences are the

spectrogram and three-dimensional power spectrum, representations

similar to those frequently used in the field of digital signal

processing. The user assigns a numerical value to each of the DNA

bases (G,C,A,T), thereby converting the string of characters to a

digitized waveform.

The user also specifies a data window (i.e., how many contiguous bases will be characterized in each strip of the

output display) and a window overlap (how many bases the adjacent

windows have in common). If the user desires to focus on smaller

regions of the DNA and is not concerned with low frequency patterns,

a small window may be chosen. If the user desires a more global

characterization of the patterns within the DNA sequence, a large

window is chosen. The overlap parameter makes it easier to capture

the spatial dynamics of the features of interest. In both the 3-D

power spectrum and spectrogram, the mean window value is subtracted,

and Hamming cosine tapers are first applied to each window of data

prior to fast Fourier transformation.

Hillocks in the three-dimensional spectrum, and darkness on spectrogram, indicate prominent

periodicities in the input sequence; the more common the periodicity,

the greater the intensity. Since both the spectrogram and 3-D power

spectrum present nucleic acid sequence data in a way which can be

visually interpreted by the molecular geneticist, a variety of

nucleotide sequence characterizations is

facilitated. This technique

has been successfully applied to detect the spatial evolution of

sequence periodicities in a human bladder cancer gene analysis.

Spectrographic representation of protein breathing motions - A

complete description of a globular protein requires not only a static

three-dimensional x-ray structure, but also an understanding of its

flexibility and the role that structural fluctuations play in the protein's function.

Globular proteins in solution exhibit a large variety of motion. As above, 3-D power spectra can be applied to the

study of such molecular motions. In particular, "low frequency"

vibrations of globular proteins, corresponding to the collective

oscillations of atoms from many different residues, can be

considered. Radii of gyration fluctuations provide a sensitive way to

characterize such concerted motions. In the current work, a research

system for the computation of digital spectrograms and topographic

spectral distribution functions of protein breathing motions was

developed.

For the topographic power spectrum (amplitude vs. frequency vs. time), hillocks are indicative of prominent

periodicities in the concerted radial motions within the protein.

When applied to a small protein (bovine pancreatic trypsin inhibitor)

a 3-D power spectrum computed for the  $R_g$  fluctuations indicates most

of the frequency power below 1 ps with a particularly prominent

breathing mode centered at 3 ps. Since both the spectrogram and 3-D

power spectrum present breathing motion data in a way which can be

easily understood by the biophysicist, characterization of the

dynamical richness of proteins is greatly facilitated. DNA Face Icon

- This visual method of data reduction is accomplished by

computer-drawn faces which function as multivariate representations

sensitive to regularities and irregularities of the statistical

properties of the sequence of bases.

Various graphical methods of representing multivariate data using icons, or symbols, have been

discussed previously. The system presented here is special in that

it has as its primary focus the rapid characterization of a

multi-dimensional data series using an interactive graphics system

with a variety of controlling parameters. In general, n data

parameters are each mapped into a figure with n features, each

feature varying in size or shape according to the point's coordinate

in that dimension. One particularly novel method of representing

multivariate data has been presented by Chernoff.

The data sample

variables are mapped to facial characteristics; thus, each

multivariate observation is visualized as a computer drawn face.

Such faces have been shown to be more reliable and more memorable

than other tested icons and allow the human analyst to grasp many of

the essential regularities and irregularities in

the data. In this disclosure, faces are used to represent statistical properties of the

sequence of bases in the DNA of a human bladder cancer gene. In order

to use the system for a DNA sequence, a file containing a listing of

the nucleic acid bases (G, C, A, T) is required. The user specifies a

window size (how many contiguous bases will be represented in each

face of the output display, e. g., 100 bases), and the program then

automatically marches through the sequence, drawing one face for each window.

In the current applications, ten facial parameters,

$F(1,2,3,4, 5,6,7,8,9,10)$ , are used, and each facial characteristic

has ten settings,  $S(1,2,3,4,5,6,7,8,9,10)$ . The simplest way to take

specific sequence interactions into account is to assume that all

effects are dominated by nearest-neighbor interactions. In this

disclosure, the occurrences of the 10 possible neighbor pairs

(GC, GA, GT, GG, CA, CT, CC, TA, TT, AA) are individually summed within a

data window, and the deviation of the sums from the expected (random)

value causes deviations of the facial parameters from their middle

positions. The computer-drawn faces were calculated and displayed

for a human bladder oncogene. The computer-drawn faces allow one to

detect substantial changes in the base composition of a gene

sequence. A massive amount of data is condensed into a small number of faces.

In summary, the icons presented in this disclosure provide

a qualitative awareness of complex DNA sequence trends, and may

subsequently guide the researcher in applying more traditional

statistical calculations. They point out regularities and

irregularities in the DNA sequence which are not easy to observe

using conventional techniques. Overall Feature Summary - Graphics are

generally limited to a finite number of dimensions, requiring that

many multivariate data problems be reduced to fewer dimensions before

analysis. The various techniques and programs described here are

useful in allowing a user to detect and comprehend important

phenomena and for communicating major conclusions to others.

What

makes the graphics system described here special is its primary focus

on the rapid characterization of a dynamic sequence of data using an

interactive graphics system with a variety of controlling parameters.

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